

A “hybrid plane” with spin-orbit interaction

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In memoriam Vladimir A. Geyler (1943-2007)

In this paper we attempt to reconstruct one of the last projects of Volodya Geyler which remained unfinished. We study motion of a quantum particle in the plane to which a halfline lead is attached assuming that the particle has spin $\frac{1}{2}$ and the plane component of the Hamiltonian contains a spin-orbit interaction of either Rashba or Dresselhaus type. We construct the class of admissible Hamiltonians and derive an explicit expression for the Green function applying it to the scattering in such a system.

1 Introduction

There is no doubt that in the person of Volodya Geyler, science lost a bright personality, somebody who with safety and elegance treaded forward at the boundary between mathematics and physics, mastering the subtleties of the former and understanding deeply the meaning of the latter. For the authors of the present paper the sad news have a personal touch because the last talk he announced bore the title *Exner-Šeba hybrid plane with the Rashba Hamiltonian*; he passed away at the opening of the conference in the Isaac Newton Institute in Cambridge where it had to be presented.

We can only guess what Volodya intended to report but we decided that the best way to honour his memory is to reconstruct what we think could be

the contents of this lecture. We take the “hybrid plane” which we introduced twenty years ago and look what happens if the particle living in it has a spin and is subject to spin-orbit interaction in the plane part of the configuration space; we consider the two interaction forms which were objects of interest recently. We construct the class of admissible Hamiltonians described by the boundary condition in the coupling point between the plane and the halfline lead attached to it. After that we derive an explicit expression for the respective Green’s functions using standard Krein’s function technique, and show how one can use them to derive properties of such system.

Since this is not intended to be an in-depth study, we will speak mostly about the simple situation when there is no external field. It is easy to extend the results to the situation when the particle is subject to a homogeneous magnetic field in the plane. We will comment on this case briefly hoping that this and other ideas related to the problem will find a continuation.

2 Spin-orbit interaction

Let us first recall how one describes a two-dimensional particle with spin-orbit interaction; as announced we will pay most attention to the simple case where there is no external field, adopting the notation from [BGP07]. For a particle with two spin states the state Hilbert space is $\mathcal{H}_{\text{plane}} = L^2(\mathbb{R}^2, \mathbb{C}^2)$ and its free motion is described by $\hat{H}_0 = \frac{1}{2m^*} \mathbf{p}^2 \sigma_0$, where $p_j = -i\hbar \partial_j$, $j = 1, 2$, as usual, and σ_0 is the 2×2 unit matrix. The spin-orbit interaction is introduced in different way: one is the so-called *Rashba Hamiltonian*

$$\hat{H}_R := \hat{H}_0 + \frac{\alpha_R}{\hbar} \hat{U}_R, \quad \hat{U}_R := \sigma_1 p_2 - \sigma_2 p_1, \quad (2.1)$$

where $\alpha_R \in \mathbb{R}$ is the Rashba constant and σ_j are the usual Pauli matrices, the other is the *Dresselhaus Hamiltonian*

$$\hat{H}_D := \hat{H}_0 + \frac{\alpha_D}{\hbar} \hat{U}_D, \quad \hat{U}_D := \sigma_2 p_2 - \sigma_1 p_1, \quad (2.2)$$

in which interaction strength is given by Dresselhaus constant $\alpha_D \in \mathbb{R}$.

Since the choice of the units will not be important in the following we get rid of the constants in the usual way introducing $\mathbf{k} := \hbar^{-1} \mathbf{p}$ and $\varkappa_j := \hbar^{-2} m^* \alpha_j$, $j = R, D$. Up to the multiplicative factor, $\hat{H}_J = \frac{\hbar^2}{2m^*} H_J$, $J = R, D$, the both versions of the Hamiltonian acquire then the simple form

$$H_J = H_0 + 2\varkappa_J U_J, \quad U_R := \sigma_1 k_2 - \sigma_2 k_1, \quad U_D := \sigma_2 k_2 - \sigma_1 k_1, \quad (2.3)$$

with $H_0 := \mathbf{p}^2 \sigma_0$, which we shall use in the following.

As usual the properties of such a Hamiltonian are encoded in its resolvent. The latter is known explicitly from the paper [BGP07]. By a nice algebraic trick, so characteristic for the work of Volodya Geyler, the derivation is reformulated as a scalar problem which involves the well know resolvent kernel $G_0(\mathbf{x}, \mathbf{x}'; z) = \frac{1}{2\pi} K_0(\sqrt{-z} |\mathbf{x} - \mathbf{x}'|)$ of the Laplacian in $L^2(\mathbb{R}^2)$, where K_0 is the zero-order MacDonald function. It leads to the expression

$$G_J(\mathbf{x}, \mathbf{x}'; z) = \begin{pmatrix} G_J^{11}(\mathbf{x}, \mathbf{x}'; z) & G_J^{12}(\mathbf{x}, \mathbf{x}'; z) \\ G_J^{21}(\mathbf{x}, \mathbf{x}'; z) & G_J^{22}(\mathbf{x}, \mathbf{x}'; z) \end{pmatrix} \quad (2.4)$$

with the diagonal elements

$$G_J^{11}(\mathbf{x}, \mathbf{x}'; z) = G_J^{22}(\mathbf{x}, \mathbf{x}'; z) = \frac{1}{4\pi} \left[-\frac{\varkappa_J}{i\sqrt{-(z + \varkappa_J^2)}} \right. \\ \left. \times (K_0(\zeta_J^+ |\mathbf{x} - \mathbf{x}'|) - K_0(\zeta_J^- |\mathbf{x} - \mathbf{x}'|)) + K_0(\zeta_J^+ |\mathbf{x} - \mathbf{x}'|) + K_0(\zeta_J^- |\mathbf{x} - \mathbf{x}'|) \right]$$

for both the $J = R, D$, while the off-diagonal ones are

$$G_R^{12}(\mathbf{x}, \mathbf{x}'; z) = \frac{i(x_2 - x'_2) - (x_1 - x'_1)}{4\pi i\sqrt{-(z + \varkappa_R^2)} |\mathbf{x} - \mathbf{x}'|} \sum_{\nu=\pm} \nu \zeta_R^\nu K_1(\zeta_R^\nu |\mathbf{x} - \mathbf{x}'|), \\ G_D^{12}(\mathbf{x}, \mathbf{x}'; z) = \frac{(x_2 - x'_2) - i(x_1 - x'_1)}{4\pi i\sqrt{-(z + \varkappa_D^2)} |\mathbf{x} - \mathbf{x}'|} \sum_{\nu=\pm} \nu \zeta_D^\nu K_1(\zeta_D^\nu |\mathbf{x} - \mathbf{x}'|),$$

and $G_J^{21}(\mathbf{x}, \mathbf{x}'; z) = \overline{G_J^{12}(\mathbf{x}', \mathbf{x}; \bar{z})}$; the effective momenta are defined at that as

$$\zeta_J^\pm := \sqrt{-(z + \varkappa_J^2)} \pm i\varkappa_J \quad (2.5)$$

For the hybrid plane model which we will describe in the next section we will need also the renormalized Green's function, i.e. the diagonal value obtained after the subtraction of the divergent term,

$$G_J^{\text{ren}}(z) := \lim_{\mathbf{x}' \rightarrow \mathbf{x}} \left[G_J(\mathbf{x}, \mathbf{x}'; z) + \frac{1}{2\pi} \ln |\mathbf{x} - \mathbf{x}'| \sigma_0 \right]; \quad (2.6)$$

notice that the limit is independent of the position \mathbf{x} in view of the translational invariance of the Hamiltonian H_J . By a straightforward computation [BGP07] one finds that the off-diagonal elements vanish in the limit while

$$G_J^{\text{ren};jj}(z) = -\frac{\varkappa_J}{2i\sqrt{-(z + \varkappa_J^2)}} (Q(\zeta^+) - Q(\zeta^-)) + \frac{1}{2} (Q(\zeta^+) + Q(\zeta^-))$$

with $Q(z) := \frac{1}{2\pi}(\psi(1) - \frac{1}{2}\ln(-z) + \ln 2)$ expressed through the digamma function, hence the renormalized Green's function can be written as

$$G_J^{\text{ren}}(z) = \frac{1}{2\pi} \left[\psi(1) - \frac{1}{2} \ln \left(-\frac{z}{4} \right) + \frac{\varkappa_J}{2i\sqrt{-(z + \varkappa_J^2)}} \ln \frac{\sqrt{-(z + \varkappa_J^2)} + i\varkappa_J}{\sqrt{-(z + \varkappa_J^2)} - i\varkappa_J} \right] \sigma_0; \quad (2.7)$$

recall that $-\psi(1) \approx 0.577$ in the above formula is Euler's number.

The case when a homogeneous magnetic field $B = \frac{\hbar c}{e}b$ perpendicular to the plane is applied is treated in a similar way. The momentum \mathbf{k} in the Hamiltonian (2.3) has to be replaced with $\mathbf{K} = \mathbf{k} - \mathbf{a}$ where $\mathbf{A} = \frac{\hbar c}{e}\mathbf{a}$ is the vector potential associated with the field, and the Zeeman term $\gamma b \sigma_3$ with $\gamma := \frac{1}{2}g_* \frac{m_*}{m_e}$ has to be added. The reduction to the scalar case works again and yields explicit expression for Green's functions [BGP07] in terms of confluent hypergeometric instead of Bessel functions.

After this preliminary, we are ready to turn to our proper subject.

3 Motion in the hybrid plane

Let us now consider that the system has a mixed dimensionality and its configuration space consists, as in [EŠ87], of a plane described above to which a halfline lead is attached; conventionally we place the junction to the origin of coordinates in the plane. As it carries the same spin $\frac{1}{2}$ particle the lead component Hilbert space is $\mathcal{H}_{\text{lead}} = L^2(\mathbb{R}_+, \mathbb{C}^2)$, and the whole state space of the system is the consequently the orthogonal sum $\mathcal{H} := \mathcal{H}_{\text{lead}} \oplus \mathcal{H}_{\text{plane}}$. The wave functions are thus of the form $\Psi = \{\psi_{\text{lead}}, \psi_{\text{plane}}\}^T$ where each of the components is a 2×1 column.

Our aim is to find the dynamics of the particle on the described configuration space. The idea of the construction is the same as in [EŠ87], and since it was used many times — let us just recall [BEG03, BG03, BGMP02, EŠ97] as a sample of this work — we can just recall briefly the scheme and describe how it applies in the present situation. We start from the decoupled operator $H^0 := H_{\text{lead}} \oplus H_J$ where the first component is the Laplacian on the halfline $H_{\text{lead}}\psi_{\text{lead}} = -\psi_{\text{lead}}''$ with Neumann boundary condition at the endpoint, and H_J is the Hamiltonian with the spin-orbit interaction discussed in the previous section. We restrict H^0 to functions which vanish in the vicinity of the junction, obtaining thus a symmetric operator of deficiency indices $(4, 4)$, and after that we seek admissible Hamiltonians among its self-adjoint extensions.

The problem differs from those mentioned above only by the presence of the spin degree of freedom and the best way to characterize the extensions is again through boundary conditions. To this aim we need the boundary values. Those on the halfline are the columns $\psi_{\text{lead}}(0+)$ and $\psi'_{\text{lead}}(0+)$. In the plane the functions from the domain of the restriction have a logarithmic singularity at the origin and the generalized boundary values $L_j(\psi_{\text{plane}})$, $j=0,1$, appear as coefficients in the expansion

$$\psi_{\text{plane}}(\mathbf{x}) = -\frac{1}{2\pi} L_0(\psi_{\text{plane}}) \ln |\mathbf{x}| + L_1(\psi_{\text{plane}}) + o(|\mathbf{x}|). \quad (3.1)$$

Using this notation we can write the sought boundary conditions as

$$\begin{aligned} \psi'_{\text{lead}}(0+) &= A\psi_{\text{lead}}(0+) + C^*L_0(\psi_{\text{plane}}), \\ L_1(\psi_{\text{plane}}) &= C\psi_{\text{lead}}(0+) + DL_0(\psi_{\text{plane}}), \end{aligned} \quad (3.2)$$

where A, C, D are 2×2 matrices, the first and the third of them Hermitian, so the matrix $\mathcal{A} := \begin{pmatrix} A & C^* \\ C & D \end{pmatrix}$ depends of sixteen real parameters as expected. It is straightforward to check that the corresponding boundary form vanishes under the condition (3.2), and therefore each fixed \mathcal{A} gives rise to a self-adjoint extension $H_{\mathcal{A}}$ of the restricted operator. Notice that the analogous boundary conditions apply also to the magnetic case mentioned in the previous section due to the same character of the singularity.

Let us further mention that the above boundary conditions are generic but do not describe all the extensions leaving out cases when the matrix \mathcal{A} is singular; this flaw can be corrected in the standard way – see, e.g., [AP05] – if one replaces (3.2) by the symmetrized form of the relation,

$$\mathcal{A} \begin{pmatrix} \psi_{\text{lead}}(0+) \\ L_0(\psi_{\text{plane}}) \end{pmatrix} + \mathcal{B} \begin{pmatrix} \psi'_{\text{lead}}(0+) \\ L_1(\psi_{\text{plane}}) \end{pmatrix} = 0, \quad (3.3)$$

where \mathcal{A}, \mathcal{B} are matrices such that $(\mathcal{A}|\mathcal{B})$ has rank four and $\mathcal{A}\mathcal{B}^*$ is Hermitean. We will restrict ourselves, however, to the case $\mathcal{B} = -I$ in the following; the same is true for the alternative form of the b.c. mentioned below.

The choice of the parameter matrix depends on the way in which the lead and the plane are connected. In particular, diagonal A, C, D correspond to the situation when the contact does not couple the spin states, and in addition, the matrices are scalar if the coupling is spin-independent. Moreover, the lead and the plane are decoupled if \mathcal{A} is block-diagonal, i.e. $C = 0$. A naïve interpretation is that C is responsible for the coupling while A and D are

point perturbations at the contact “from the two sides”. The reality is more complicated, though. If the halfline models a thin fibre of radius ρ coupled to the plane, then in the spin-indepdent case the natural choice seem to be

$$A = \frac{1}{2\rho} \sigma_0, \quad C = \frac{1}{\sqrt{2\pi\rho}} \sigma_0, \quad D = -\sigma_0 \ln \rho \quad (3.4)$$

in analogy with the discussion of then spinless case performed in [EŠ97].

4 The Green function

Having defined the class of admissible Hamiltonians we can proceed to construction of their resolvents. One can use the standard procedure based Krein’s formula – see, e.g., [AGHH] or [BGMP02]. The starting point is Green function of the decoupled system which has a block-diagonal form,

$$G^0(x, x'; \mathbf{x}, \mathbf{x}'; z) = \begin{pmatrix} G_{\text{lead}}(x, x'; z) & 0 \\ 0 & G_{\text{J}}(\mathbf{x}, \mathbf{x}'; z) \end{pmatrix}, \quad (4.1)$$

where $G_{\text{J}}(\mathbf{x}, \mathbf{x}'; z)$ is given by (2.4) and

$$G_{\text{lead}}(x, x'; z) = \frac{i}{\sqrt{z}} \cos \sqrt{z} x_{<} e^{-i\sqrt{z} x_{>}} \sigma_0$$

with the conventional notation, $x_{<} := \min\{x, x'\}$, $x_{>} := \max\{x, x'\}$, since we assumed Neumann boundary condition. The Krein function $Q(z)$, which is an analytic 4×4 -matrix valued function of the spectral parameter z , is defined through diagonal values of the kernel, with the above described renormalization in the plane component, specifically

$$Q(z) := \begin{pmatrix} \frac{i}{\sqrt{z}} \sigma_0 & 0 \\ 0 & G_{\text{J}}^{\text{ren}}(z) \end{pmatrix}. \quad (4.2)$$

To express the full Green function it is useful to cast the conditions of the previous section into an alternative form by changing the basis in the boundary value space: instead of the vectors appearing in (3.3) we consider

$$\tilde{\Gamma}_1 \psi := \begin{pmatrix} -\psi'_{\text{lead}}(0+) \\ L_0(\psi_{\text{plane}}) \end{pmatrix}, \quad \tilde{\Gamma}_2 \psi := \begin{pmatrix} \psi_{\text{lead}}(0+) \\ L_1(\psi_{\text{plane}}) \end{pmatrix}.$$

It is easy to see that they satisfy $\tilde{\mathcal{A}}\tilde{\Gamma}_1\psi + \tilde{\mathcal{B}}\tilde{\Gamma}_2\psi = 0$ with $\tilde{\mathcal{B}} = -I$ and

$$\tilde{\mathcal{A}} := \begin{pmatrix} -A^{-1} & -A^{-1}C^* \\ -CA^{-1} & D - CA^{-1}C^* \end{pmatrix}. \quad (4.3)$$

It is obvious that $\tilde{\mathcal{A}} = -\tilde{\mathcal{A}}\tilde{\mathcal{B}}^*$ is Hermitean; we have to suppose, of course, that the matrix A is regular, or roughly speaking, that $H_{\mathcal{A}}$ has no Neumann component on the halfline (notice that this is true, e.g., for (3.4)). The advantage of these boundary conditions is that our comparison operator H^0 is characterized by $\tilde{\Gamma}_1\psi = 0$, i.e. $\tilde{\mathcal{A}}^0 = I$, $\tilde{\mathcal{B}}^0 = 0$. In such a case we can use the result of [AP05] (which in our case boils down to the usual Krein's formula) by which the resolvent kernel of $H_{\mathcal{A}}$ is given by

$$G_{\mathcal{A}}(x, x'; \mathbf{x}, \mathbf{x}'; z) = G^0(x, x'; \mathbf{x}, \mathbf{x}'; z) - G^0(x, 0; \mathbf{x}, \mathbf{0}; z) [Q(z) - \tilde{\mathcal{A}}]^{-1} G^0(0, x'; \mathbf{0}, \mathbf{x}'; z) \quad (4.4)$$

differing from the free one by the second term on the right-hand side which is a rank sixteen operator. Notice that even if the coupling is spin-independent, $\mathcal{A} = \begin{pmatrix} a & \bar{c} \\ c & d \end{pmatrix} \otimes \sigma_0$ and similarly for $\tilde{\mathcal{A}}$, the Green function does not decompose because spin states are coupled by the spin-orbit interaction in the plane.

5 Properties of $H_{\mathcal{A}}$

We will concentrate on the case when there is a nontrivial coupling between the two parts of the configuration manifold, i.e. \mathcal{A} is no block-diagonal. In the opposite case we have two separate problems; the halfline one is trivial while spin-orbit Hamiltonians with point interactions deserve an investigation – we believe that the reader can find a study on this topic in the contribution of K. Pankrashkin to this issue. To keep things simple, we suppose that the coupling is spin-independent, $\mathcal{A} = \begin{pmatrix} a & \bar{c} \\ c & d \end{pmatrix} \otimes \sigma_0$ with $c \neq 0$, so

$$Q(z) = \begin{pmatrix} \frac{i}{\sqrt{z}} - \tilde{a} & -\tilde{c} \\ -\tilde{c} & G_{\text{J}}^{\text{ren}}(z) - \tilde{d} \end{pmatrix} \otimes \sigma_0. \quad (5.1)$$

Let us first remark that the junction can bind. For instance, to any number in $(-\kappa_{\text{J}}^2, 0)$ one can find $H_{\mathcal{A}}$ for which it is an eigenvalue. Indeed, writing the negative energy as $-\kappa^2$ we see that (5.1) is singular if the relation $(\kappa^{-1} - \tilde{a})(G_{\text{J}}^{\text{ren}}(-\kappa^2) - \tilde{d}) = |\tilde{c}|^2$ is valid, or in the original parameters

$$(\kappa - a)(G_{\text{J}}^{\text{ren}}(-\kappa^2) - d) = |c|^2. \quad (5.2)$$

By (2.7) $G_J^{\text{ren}}(-\kappa^2)$ is real-valued for $\kappa^2 < \kappa_J^2$, then it is easy to pick the parameters a, d in such a way that (5.2) is satisfied.

The most interesting aspect of the problem, of course, is the transport through the junction. A straightforward way to treat it is to use the formula (4.4). Any vector of \mathcal{H} can be written as $(H^0 - z)^{-1}\psi^0$ for $\psi^0 \in D(H^0)$ and $\text{Im } z \neq 0$, hence applying the formula to it we get

$$\psi = \psi^0 - \gamma_z[Q(z) - \mathcal{A}]^{-1}\gamma_z^*(H^0 - z)^{-1}\psi^0, \quad (5.3)$$

where $\gamma_z : \mathbb{C}^4 \rightarrow \mathcal{H}$ is the trace operator given by the kernel $G^0(x, 0; \mathbf{x}, \mathbf{0}; z)$ and γ_z^* is its adjoint. Notice that $\Gamma(\bar{z})^*(H^0 - z)^{-1}\psi^0$ is just the vector of the values of ψ^0 at the connection point and $Q(z) - \mathcal{A}$ is position-independent, so the second term at the right-hand side is easy to compute. Now we employ the usual trick letting z to approach a real value k^2 . The resulting function ceases to be L^2 , of course, but it still satisfies locally the boundary conditions in the junction and it can yield a generalized eigenfunction associated with the scattering which we are looking for.

In particular, we can choose the vector ψ^0 with the “upper” component only, $\psi_{\text{plane}}^0 = 0$ and $\psi_{\text{lead}}^0 = \cos kx$ (notice that not every combination of $e^{\pm ikx}$ will do since ψ_{lead}^0 has to satisfy Neumann boundary condition at the origin). It is a straightforward exercise to invert the matrix (5.1) and to compute ψ ; it yields the reflection amplitude of a particle travelling over the halfline towards the junction with a momentum k in the form

$$\mathcal{R}(k) = \frac{\left(-\frac{i}{k} - \tilde{a}\right) (G_J^{\text{ren}}(k^2) - \tilde{d}) - |\tilde{c}|^2}{\left(\frac{i}{k} - \tilde{a}\right) (G_J^{\text{ren}}(k^2) - \tilde{d}) - |\tilde{c}|^2},$$

naturally independent of the particle spin state. It is straightforward to recompute it in terms of the original parameters from (3.2); we get

$$\mathcal{R}(k) = -\frac{(a + ik)(G_J^{\text{ren}}(k^2) - d) + |c|^2}{(a - ik)(G_J^{\text{ren}}(k^2) - d) + |c|^2}. \quad (5.4)$$

Since $G_J^{\text{ren}}(k^2)$ is generally complex $|\mathcal{R}(k)|^2$ is not equal to one for $|c| \neq 0$ which is natural because the coupling allows the particle to pass from the lead to the plane. In particular, in the absence of the spin-orbit coupling when the last term at the right-hand side of (2.7) is missing, (5.4) reduces to the reflection amplitude derived in [EŠ87] for spinless case (up to the sign of k which is due to the opposite halfline orientation used there).

In the magnetic case one can proceed in the same way replacing $G_J^{\text{ren}}(k^2)$ by the renormalized magnetic Green's function of [BGP07]. There is a substantial difference, though. Now the Green function is real-valued, and consequently, the scattering on the halfline is unitary, $|\mathcal{R}(k)|^2 = 1$. The scattering in such a case will naturally exhibit resonances due to the discrete spectrum of the spin-orbit Hamiltonian in the plane which are worth of investigation, however, this is a subject for another paper.

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